Ecotox Report for Case # P-19-0002

General

Status Date: ██████ 12/10/2018	**Report Status:** Complete
	CRSS Date: 10/29/2018
SAT Date:	**SAT Chair:**
Consolidated PMN: N	**Consolidated Set:**
Ecotox Related Cases:	
Health Related Cases:	
Submitter: ██████	
CAS Number: ██████	
Chemical Name: ██████	
Use: Chemical intermediate ██████	
Trade Name: None	
PV-max(kg/yr): ██████	**Ecotox Assessor:** Koehrn, Kara

Fate Summary Statement

Fate Summary Statement: P-19-0002
FATE:

██████ with MP = ██████ °C (M)
log Kow = 4.35 (E)
S = 1.28 mg/L
at 25 °C (E)
VP < 1.0E-6 torr at 25 °C (E)
BP > 400 °C
(E)
H < 1.00E-8 (E)
log Koc = 7.08 (E)
log Fish BCF = 0.50 (3)
(E)
log Fish BAF = 2.40 (250) (E)
POTW removal (%) = 90 via

sorption and biodeg
Time for complete ultimate aerobic biodeg =
wk
Sorption to soils/sediments = strong
PBT Potential: P2B1
FATE:
Migration to ground water = negl
Bioconcentration factor to be put into
E-FAST: 3

Physical Chemical Information

Molecular Weight:	███		
Wt% < 500:		**Wt% < 1000:**	
Physical State - Neat:	███		
Melting Point:	████	**Melting Point (est):**	
MP (EPI):			
Vapor Pressure:		**Vapor Pressure (est):**	<0.000001
VP (EPI):			
Water Solubility:		**Water Solubility (est):**	0.00128
Water Solubility (EPI):			
Henry's Law::			
Log Koc:		**Log Koc (EPI):**	
Log Kow:		**Log Kow (EPI):**	
Log Kow Comment:			

SAT Concern Level

Ecotox Rating (1):	1
Ecotox Rating Comment (1):	
Ecotox Rating (2):	
Ecotox Rating Comment (2):	

Ecotox Route of Exposure:	No releases to water

Ecotox Comments

Exposure Based Review (Eco):	N
Ecotox Comments:	
Exposure Based Testing:	

PBT Ratings

Persistence	Bioaccumulation	Toxicity	Comments
2	1		

Eco-Toxicity Comment:

Fate Ratings

Removal in WWT/POTW (Overall):	90					
Condition	Rating Values	Rating Description				Comment
		1	2	3	4	
Fish BCF:						
Log Fish BCF:						
WWT/POTW Sorption:	2-3	Low	Moderate	Strong	V. Strong	
WWT/POTW Stripping:	4	Extensive	Moderate	Low	Negligible	
Biodegradation Removal:	2	Unknown	High	Moderate	Negligible	
Biodegradation Destruction:		Unknown	Complete	Partial	—	
Aerobic Biodeg Ult:	2	<= Days	Weeks	Months	> Months	
Aerobic Biodeg Prim:		<= Days	Weeks	Months	> Months	
Anaerobic Biodeg Ult:	3	<= Days	Weeks	Months	> Months	
			Weeks	Months	> Months	

Removal in WWT/POTW (Overall):	90				
Condition	Rating Values	Rating Description			Comment
		1	2	3	4
Anaerobic Biodeg Prim:		<= Days			
Hydrolysis (t1/2 at pH 7,25C) A:		<= Minutes	Hours	Days	>= Months
Hydrolysis (t1/2 at pH 7,25C) B:		<= Minutes	Hours	Days	>= Months
Sorption to Soils/Sediments:	2	V. Strong	Strong	Moderate	Low
Migration to Ground Water:	1	Negligible	Slow	Moderate	Rapid
Photolysis A, Direct:		Negligible	Slow	Moderate	Rapid
Photolysis B, Indirect:		Negligible	Slow	Moderate	Rapid
Atmospheric Ox A, OH:		Negligible	Slow	Moderate	Rapid
Atmospheric Ox B, O3:		Negligible	Slow	Moderate	Rapid
Bio Comments:	Fish log BAF = 2.40 (250). The fugacity spreadsheet and the EPI output file for the PMN material are attached.				
Fate Comments:					

Ecotoxicity Values

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	96-h	LC50	>100		Predictions are based on QSARs for neutral organics (ECOSAR V2.0)
Daphnid	48-h	LC50	>100		" "
Green Algae	96-h	EC50	>100		" "

Test organism	Test Type	Test Endpoint	Predicted	Experimental	Comments
Fish	-	Chronic Value	>10		" "
Daphnid	-	Chronic Value	>10		" "
Green Algae	-	Chronic Value	>10		" "

Ecotox Value Comments: Predictions are based on QSARs for neutral organics (ECOSAR V2.0); MW ███ ; Log Kow = 0.54 (P); ███ with a MP = ████ C (M);
S = 142 mg/L (P); effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <150 mg/L as CaCO3; and TOC <2.0 mg/L. We used the following smiles to account for the fact that this is a charged molecule.
███████████████████

Ecotox Factors

Factors	Most Sensitive Endpoint	Assessment Factor	CoC	Comment
Acute Aquatic (ppb):	100,000	5	20,000	based on acute fish ECOSAR predictions
Chronic Aquatic(ppb):	10,000	10	1,000	based on chronic fish ECOSAR predictions

Factors	Values	Comments
SARs:	Neutral Organics	
SAR Class:	Neutral organics-aromatic tetraacid	
TSCA NCC Category?	Neutral Organics	

Recommended Testing:

Ecotox Factors Comments: Environmental Hazard: Environmental hazard is relevant to whether a new chemical substance is likely to present unreasonable risk because the significance of the risk is dependent upon both the hazard (or toxicity) of the chemical substance and the extent of exposure to the substance. EPA estimated environmental hazard of this new chemical substance using the Ecological Structure Activity Relationships (ECOSAR) Predictive Model

(https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-releationships-ecosar-predictive-model);
specifically the QSAR for neutral organics. This substance falls within the TSCA New Chemicals Category neutral organics. Acute toxicity values estimated for fish, aquatic invertebrates, and algae are >100 mg/L. Chronic toxicity values estimated for fish, aquatic invertebrates, and algae are >10 mg/L. These toxicity values indicate that the new chemical substance is expected to have low environmental hazard. Application of assessment factors of 5 and 10 to acute chronic toxicity values, respectively, results in an acute concentration of concern of 20.0 mg/L (20,000 ppb) and a chronic concentration of concern of 1.0 mg/L (1,000 ppb).

Environmental Risk: Risks to the environment were evaluated by comparing estimated surface water concentrations with the acute and chronic concentrations of concern. Acute and chronic risks to the environment were not identified due to releases to water that did not exceed the acute nor the chronic COC.

Comments/Telephone Log

Artifact	Update/Upload Time